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On a Generalization of the Hermite Constant

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Abstract. We report some results on the theory of quasiperiodic sphere packings controlled by a finite group G in the n -dimensional Euclidean space, constructed by means of an higher dimensional Euclidean space which contains G -invariant lattices. A generalization of the Hermite constant is used to find upper bounds of the density.

1. Introduction

We will study a density function associated with some quasiperiodic sphere packings $\mathcal{K}_Q(\Lambda)$ in the n -dimensional Euclidean space $\mathbb{E}^n = (\mathbb{R}^n, \|\cdot\|)$, $n \geq 1$, obtained from lattices Λ in higher-dimensional spaces $\mathbb{E}^k$, $k > n$, controlled in some sense by a finite group G , and look for densest such quasiperiodic sphere packings and their densities. By quasiperiodic sphere packing, we mean that all the centers of spheres are on a finite rank $\mathbb{Z}$ -module in $\mathbb{E}^n$. This density function will arise from a generalization of the Hermite constant. Recall at first the standard terminology of sphere packing theory to fix some notations [1, 2, 3].

Let $\mathbb{B}_n(r)$ the n -dimensional closed ball of volume $v_n(r) = \pi^{n/2} r^n / \Gamma(\frac{n+2}{2})$, centred at the origin, of radius $r > 0$, called traditionally “sphere”, in $\mathbb{E}^n$. For any discrete (periodic or not) set of points $\{a_i\}_{i \in \mathbb{N}}$ in $\mathbb{E}^n$, we will assume that there exists a constant $T > 0$ such that, for each $x \in \mathbb{E}^n$, there exists an i such that $\|x - a_i\| < T$, and we will consider the system of spheres $\mathcal{K} = \{a_i + \mathbb{B}_n(r)\}$ such that the common value r is chosen as large as possible such that the balls $\{a_i + \mathbb{B}_n(r)\}$ have pairwise disjoint interiors. Let us call $\delta(\mathcal{K})$ its global density, defined by

$$(1) \quad \delta(\mathcal{K}) = \limsup_{R \rightarrow +\infty} \left[\text{vol} \left(\left(\bigcup_i (a_i + \mathbb{B}_n(r)) \right) \cap \mathbf{B}(0, R) \right) / \text{vol}(\mathbf{B}(0, R)) \right]$$

To each sphere $a_i + \mathbb{B}_n(r)$ in $\mathcal{K}$ is associated its local cell $\mathbf{C}(a_i, \mathcal{K})$ defined by the closed convex polyhedron

$$(2) \quad \mathbf{C}(a_i, \mathcal{K}) = \{x \in \mathbb{E}^n / \|x - a_i\| \leq \|x - a_j\| \text{ for all } j \neq i\}$$

and its local density $\Delta(a_i, \mathcal{K})$ at a_i

$$(3) \quad \Delta(a_i, \mathcal{K}) = v_n(r)/\omega_i$$

where $\omega_i = \text{vol}(C(a_i, \mathcal{K}))$. The decomposition into Voronoi polyhedra of the sphere packing forms a tiling. The above assumption, on the existence of T , will ensure that each local tile is bounded, that the packing of spheres thus obtained remains fairly uniform from the point of view of the density, in every direction in space. The global density $\delta(\mathcal{K})$ is then the weighted average of the local densities $\Delta(a_i, \mathcal{K})$, where the weights are the ω_i 's, all strictly positive. Upper bounds for local densities are consequently upper bounds for the global density. Let us call $\delta_n = \sup_{\mathcal{K}} \delta(\mathcal{K})$ the packing constant of $\mathbb{B}_n(1)$, (resp. $\delta_{L,n}$, resp. $\delta_{P,n}$) where the supremum is taken over all possible sphere packings systems $\mathcal{K}$ in $\mathbb{E}^n$, (resp. sphere packings systems for which the centers a_i form a lattice, the supremum being taken over all lattices in $\mathbb{E}^n$; resp. sphere packings systems for which the centers a_i form a crystal (*periodic system* in the sense of [1], p. 25), the supremum being taken over all crystals in $\mathbb{E}^n$). Going from any $r > 0$ to $r = 1$ for the radius of the balls does not change anything in the definition of the maximal densities because of Theorem 1.7 in [1]. Rogers [1] proved

$$(4) \quad \delta_{L,n} \leq \delta_{P,n} = \delta_n$$

and therefore, we do not gain in maximal density going from sphere crystals to non periodic systems of spheres in general.

In dimension 2, Thue (1910) [4] and L. Fejes Tóth (1940) [5] have proved that the densest packing of circles is obtained from a lattice packing (hexagonal packing $\mathcal{K}$) with $\delta_2 = \delta_{L,2} = \delta(\mathcal{K}) = \Delta(a_i, \mathcal{K}) = \pi/\sqrt{12} = 0.9069\dots$ (Lagrange, Gauss [6, 7]); geometrically, the plane can be tiled with regular triangles. In dimension 3, several authors have computed upper bounds for the local densities: (1929) Blichfeldt [8]: $0.835\dots$; (1958) Rogers [1]: $\sigma_3 = \sqrt{2}(3\text{Arccos}(\frac{1}{3}) - \pi) = 0.7796\dots$; (1986) Lindsey [9]: $0.77844\dots$; (1988, 1993) Muder [10]: $0.77836\dots$, then $0.773055\dots$. Here, σ_h denotes, in a regular simplex in $\mathbb{R}^h$ with $h+1$ vertices, the ratio of the volume occupied by the $h+1$ (tangent) spheres centered at the vertices to the volume of the whole simplex. In dimension $n \geq 2$, Rogers [1] proved ingeniously that the packing constant always satisfies $\delta_n \leq \sigma_n$. Hsiang (1993) [11] claimed the proof of the upper bound of the local density: $\frac{4\pi}{3} : 20(1 - 2\cos\frac{2\pi}{5})\tan\frac{\pi}{5} = 0.75469\dots$, in a very controversial and incomplete paper [13, 15, 16] where some results are wrong, in an attempt to also prove Kepler's conjecture, which states that

$$(5) \quad \delta_3 = \delta_{L,3} = \pi/\sqrt{18}$$

and this proof of the value of this upper bound is considered as not established, as well as Kepler's conjecture [17].

L. Fejes Tóth conjectured [18, 19, 20] that the optimal upper bound of the local density $0.75469\dots$ in $\mathbb{E}^3$ can be realized when the configuration of the first neighbor spheres is an icosahedron, what says that the corresponding optimal local cell, as the smallest volume Voronoi polyhedron, is a regular dodecahedron. Hales [12, 13, 14], in a five-step program, attempts to overcome all the difficulties

encountered by Hsiang by different techniques, and proposes a resolution scheme for proving Kepler's conjecture based on nonlinear optimization problems. More recently, K. Bezdek [16] reexpressed this conjecture of L. Fejes Tóth about the optimal Voronoi cell as the *Dodecahedral Conjecture*, relating it to others conjectures, namely a so-called *Conjecture A*, a *Distance Conjecture* and an *Isoperimetric Conjecture*. The central fact, in the scope to make a link with tilings, is that this optimal cell — a regular dodecahedron — cannot tile periodically, as a unique prototile, the 3-dimensional Euclidean space. To study the infinitely many possible local configurations of spheres, within a fairly narrow zone of influence about each sphere (center-distance from the central sphere less than $2.18 \times$ common radius of the spheres), Hsiang used the notion of *locally averaged density* associated with the Voronoi decomposition. Hales relates the Delaunay decomposition and gives upper estimates for the *score*, a function which also measures the averaged local density, associated with this decomposition, or with a mixed decomposition Voronoi+Delaunay. Functions over Voronoi cells or Delaunay decompositions, or mixed decompositions, generalizing the $\Delta(a_i, \mathcal{K})$ are now essential.

In each case ($n = 2$ and 3), a symmetry group (C_3 and resp. the icosahedral group) intervenes in the geometry of the optimal Voronoi cell, together with the possibility of tiling space periodically or not with it. In the following, we will consider the reverse situation and we will start from a finite group. This finite group, say G , assumed non trivial, will give rise to quasiperiodic sphere packings $\mathcal{K}_Q(\Lambda) = \{a_i + \mathbb{B}_n(r)\}$ in $\mathbb{E}^n$ associated with it, obtained from lattices Λ in higher-dimensional Euclidean spaces $\mathbb{E}^k$, for suitable values of $k > n$, by a continuous selection process by a *window* in $\mathbb{R}^{k-n}$. Their Voronoi cells will be reinvestigated afterwards by local, locally averaged densities or scores. Whatever Λ , this group G , and the window, will control in some sense the possible local configurations of Voronoi cells in $\mathcal{K}_Q(\Lambda)$ and their frequencies of occurrence. If Fejes Tóth's conjecture is true, the optimal Voronoi cell in dimension 3 is invariant under the icosahedral group, and we take as G the icosahedral group. We could conjecture that in dimension $n \geq 4$ arbitrary, the smallest Voronoi polyhedron of a sphere packing is also invariant under a finite symmetry group, say G_n . We take in the above constructions $G = G_n$. In §2, we indicate a possible arithmetical construction for k associated with G -invariant lattices in $\mathbb{R}^k$. In §3, we give the method of construction we follow of quasiperiodic sphere packings, and introduce a generalized Hermite function.

What can we expect from such quasiperiodic configurations ? Since possibly $\delta_{L,n} < \delta_n$ from (4), do such densest quasiperiodic systems of spheres give intermediate values between $\delta_{L,n}$ and δ_n ? What is the maximal density $\delta_{Q,n}^{(k)}$ of quasiperiodic packing systems of spheres in $\mathbb{E}^n$ when k is fixed ? What is the maximal density $\delta_{Q,n}$ of quasiperiodic packing systems of spheres in $\mathbb{E}^n$, over all values of k ? In this contribution, we limit ourselves to give an upper bound of $\delta_{Q,n}^{(k)}$, in §4.

In §5, we indicate a few examples associated with Penrose tilings concerned with some space-filling problems in crystallography and modelling of quasicrystals in physics [28]. Quasiperiodic sphere packings were considered by several authors in different contexts, for instance [21, 22, 23, 24, 25, 26]. We will review some ef-

fective constructions of quasiperiodic systems of spheres and indicate the respective densities.

2. A construction

PROPOSITION 1. *Let G a non trivial finite group, $\rho : G \rightarrow GL_n(\mathbb{R})$, a real linear faithful representation of G , then there exists an integer $k \geq n$, a linear faithful representation $\tilde{\rho} : G \rightarrow GL_k(\mathbb{R})$ and an embedding $j : \mathbb{R}^n \rightarrow \mathbb{R}^k$ such that*

$$(6) \quad \forall g \in G, \forall x \in \mathbb{R}^n, \tilde{\rho}(g)(j(x)) = j(\rho(g)(x))$$

and $\mathbb{R}^k$ contains $\tilde{\rho}(G)$ -invariant lattices. $j(\mathbb{R}^n)$ is orthogonal direct factor in $\mathbb{R}^k$ and the orthogonal projector $\pi_{\parallel} : \mathbb{R}^k \rightarrow j(\mathbb{R}^n)$ commutes with the action of G , namely

$$(7) \quad \forall g \in G, \forall y \in \mathbb{R}^k, \pi_{\parallel}(\tilde{\rho}(g)(y)) = j(\rho(g)\pi_{\parallel}(y)).$$

PROOF This result should be classical. A construction could be the following one. Since G is finite, and the representation ρ real, there exists a real number field K , of degree say $d \geq 1$, $d = [K : \mathbb{Q}]$, and a basis of $\mathbb{R}^n$ such that the matrices $M(g)$ of the operators $\rho(g)$ expressed in this basis have all their entries in K [29]. This basis allows K^n to be embedded in $\mathbb{R}^n$ as a $(\rho(G)$ -invariant) G -invariant module. Denoting by $\mathcal{O}_K$ the ring of integers of K , which is a free $\mathbb{Z}$ -module of rank d in K , any $\mathcal{O}_K$ -module $\mathcal{L}$ of rank n in K^n , gives a $\rho(G)$ -invariant free module of rank nd over $\mathbb{Z}$

$$(8) \quad \mathcal{L}^{(G)} = \bigcap_{g \in G} \rho(g)(\mathcal{L})$$

But K is canonically embedded in $\mathbb{R}^{r_1} \times \mathbb{C}^{r_2}$ by the injective ring homomorphism

$$\begin{aligned} \sigma : K &\rightarrow \mathbb{R}^{r_1} \times \mathbb{C}^{r_2} : x \rightarrow \sigma(x) \\ &= (\sigma_1(x), \sigma_2(x), \dots, \sigma_{r_1}(x), \sigma_{r_1+1}(x), \sigma_{r_1+2}(x), \dots, \sigma_{r_1+r_2}(x)) \end{aligned}$$

where $\sigma_1, \sigma_2, \dots, \sigma_{r_1}, \sigma_{r_1+1}, \bar{\sigma}_{r_1+1}, \sigma_{r_1+2}, \bar{\sigma}_{r_1+2}, \dots, \sigma_{r_1+r_2}, \bar{\sigma}_{r_1+r_2}$ are the real and complex canonical embeddings of K in $\mathbb{R}$ and $\mathbb{C}$, with $d = r_1 + 2r_2$. We identify $\mathbb{R}^{r_1} \times \mathbb{C}^{r_2}$ with $\mathbb{R}^d$. Defined component by component, the injective ring homomorphism $\sigma^{(n)} : K^n \rightarrow (\mathbb{R}^{r_1} \oplus \mathbb{C}^{r_2})^n : (x_1, x_2, \dots, x_n) \rightarrow (\sigma(x_1), \sigma(x_2), \dots, \sigma(x_n))$ sends $\mathcal{L}^{(G)}$ onto a $\mathbb{Z}$ -lattice $\sigma(\mathcal{L}^{(G)}) \subset \mathbb{R}^{nd}$ of rank nd . Since $\mathcal{L}^{(G)}$ is $\rho(G)$ -invariant and $\sigma^{(n)}$ injective, the action of G on K^n leads to an action on the image $\sigma(\mathcal{L}^{(G)})$, which is therefore G -invariant, that is an action on $\mathbb{R}^{nd}$ (working with full rank $\mathbb{Z}$ -modules), which corresponds to a faithful linear representation $\tilde{\rho}$, with $k = nd$. Since K is assumed real, $r_1 \geq 1$, we can take the first real component of $\mathbb{R}^{nd} = \mathbb{R}^n \times \mathbb{R}^{n(r_1-1+2r_2)}$ for the initial representation space of dimension n on which G acts through ρ . This defines an injective application j , compatible with the two actions of G as given in eq. (6), embedding $\mathbb{R}^n$ into $\mathbb{R}^k$ as $\mathbb{R}[G]$ -modules. The Frobenius-Schur Theorem [29] gives the scalar product of $\mathbb{R}^{nd}$ as $\tilde{\rho}(G)$ -invariant and the orthogonality of the $\mathbb{R}[G]$ -submodules of $\mathbb{R}^k$. Eq. (7) is deduced from eq. (6). $\square$

REMARK 1. It is clear that there exists a minimal value of k allowing such constructions, which corresponds to a finite number of number fields extensions $K/\mathbb{Q}$. If $k = n$, this means that G is compatible with a lattice, and that it is a subgroup of the holohedry group of a lattice. We will be interested in the following in sphere packings in $\mathbb{E}^n$ which are not periodic, that is for values of k strictly greater than n , centers of spheres lying on a $\mathbb{Z}$ -module of rank k .

REMARK 2. The classification of G -invariant lattices in dimension k with the possible types of groups G amounts to find all the conjugacy classes of finite subgroups of $GL(k, \mathbb{Z})$, the group of integral $k \times k$ matrices with determinant ± 1 . This number of classes is finite by the Jordan–Zassenhaus Theorem [30]. In small dimension, explicit results are known [31, 32, 33, 34, 35, 36, 37, 38, 39] and, for general k values, an algorithm was developed by Plesken [40].

3. Quasiperiodic sphere packings

If Λ denotes a lattice in $\mathbb{R}^k = \mathbb{E}^n \oplus \mathbb{R}^{k-n}$, we will consider sphere packing systems $\mathcal{K}_{\mathbb{Q}}^k(\Lambda) = \{a_i + \mathbb{B}_n(r)\}$ in $\mathbb{E}^n$ such that for all $i, a_i \in \pi_{\parallel}(\Lambda)$; the rank of this quasiperiodic system of spheres is k . As a $\mathbb{Z}$ -module, we know that $\pi_{\parallel}(\Lambda)$ can be decomposed into two $\mathbb{Z}$ -modules $\pi_{\parallel}(\Lambda) = \mathcal{L}_1^{\parallel}(\Lambda) \oplus \mathcal{L}_2^{\parallel}(\Lambda) \subset \mathbb{E}^n$, the first one which is dense and the second one discrete (and chosen in a non canonical way), such that, if d_1 and d_2 denote the respective dimensions of the affine subspaces generated by $\mathcal{L}_1^{\parallel}(\Lambda)$ and $\mathcal{L}_2^{\parallel}(\Lambda)$, we have $n = d_1 + d_2$. Since k is assumed $> n$, we have always $d_1 \geq 1$. If $d_2 \geq 1$, the quasiperiodic sphere packing will be quasiperiodic in “ d_1 directions”, and partially periodic in “ d_2 directions”. If $d_1 = n$, it is said *purely quasiperiodic*. For any lattice Λ in $\mathbb{R}^k$, the two following quantities are intrinsically defined, that is independant of the choice of a basis in Λ : the minimal square norm

$$(9) \quad m^{(k)}(\Lambda) = \inf_{x \in \Lambda, x \neq 0} \langle x, x \rangle$$

where $\langle, \rangle$ denotes the standard scalar product; if $\{x_i\}_{0 \leq i \leq k}$ is an arbitrary basis of Λ , the discriminant

$$(10) \quad \text{disc}(\Lambda) = \det(\langle x_i, x_j \rangle)$$

As usual, we set

$$(11) \quad \gamma^{(k)}(\Lambda) = \frac{m^{(k)}(\Lambda)}{\text{disc}(\Lambda)^{1/k}}.$$

When Λ describes the locally compact space of all the lattices in $\mathbb{R}^k$, which can be parametrized by $GL_k(\mathbb{R})/GL_k(\mathbb{Z})$, the function $\Lambda \rightarrow \gamma^{(k)}(\Lambda)$, which is continuous, proper, reaches its maxima and its minima [2]. We call $\gamma_k = \sup_{\Lambda} \gamma^{(k)}(\Lambda)$ the *Hermite constant* in dimension k .

We now turn to quasiperiodic systems of spheres. At first, we define a *selection mode* (or a *window*) on the elements of Λ , in $\mathbb{R}^{k-n}$, the space orthogonal to $\mathbb{E}^n$ in $\mathbb{R}^k$,

to keep only an infinite Delaunay set of points in $\mathbb{E}^n$ satisfying the uniform density assumption (§1: existence of T) in $\pi_{\parallel}(\Lambda)$. This selection mode is the following: we start from a reduction scheme (using a reduction theory [42]: Minkowski, Korkin–Zolotarev, Selling, etc), that we call $\mathcal{R}(\Lambda)$, to find a $\mathbb{Z}$ -reduced basis $\{z_1, z_2, \dots, z_k\}$ in Λ . Second, with $\pi_{\perp} = Id - \pi_{\parallel}$, we call

$$(12) \quad W_{\mathcal{R}(\Lambda)} = \pi_{\perp} \left(\left\{ \sum_{t=1}^k \lambda_t z_t \mid \forall t = 1, 2, \dots, k, 0 \leq \lambda_t \leq 1 \right\} \right)$$

the *window* associated with $\mathcal{R}(\Lambda)$ and $\{z_1, z_2, \dots, z_k\}$. It is a convex polytope, and let $\mathbb{R}^{k-n}$ be its affine hull. We form the subset

$$(13) \quad \mathcal{K}_{\mathbb{Q}, \mathcal{R}, \{z_i\}}^k(\Lambda) = \{\pi_{\parallel}(c_i) + \mathbb{B}_n(r) \mid c_i \in \Lambda, \pi_{\perp}(c_i) \in \overset{\circ}{W}_{\mathcal{R}(\Lambda)}\}$$

denoted in a simpler way $\mathcal{K}_{\mathbb{Q}}^k(\Lambda)$, with a radius r for the spheres centred at the $\pi_{\parallel}(c_i)$'s taken maximal to have a packing, and with a selection with the interior $\overset{\circ}{W}_{\mathcal{R}(\Lambda)}$ of the window. It is clear that for some lattices Λ , the common value r will be extremely small, and the density very low.

LEMMA 1. *Two distinct points x and y of Λ such that $\pi_{\perp}(x), \pi_{\perp}(y) \in \overset{\circ}{W}_{\mathcal{R}(\Lambda)}$ cannot project by $\pi_{\parallel}$ on the same element in $\pi_{\parallel}(\Lambda)$.*

This is due to the fact that the reduction process provides minimal norm vectors [41, 42], and that if an element $v \in \Lambda \cap \overset{\circ}{W}_{\mathcal{R}(\Lambda)}$, it should have been taken as an element of the basis $\{z_i\}$.

LEMMA 2. *For any compact set $C \subset \mathbb{E}^n$ the number of elements in*

$$(14) \quad \{x \in \Lambda \mid \pi_{\parallel}(x) \in C \text{ and } \pi_{\perp}(x) \in \overset{\circ}{W}_{\mathcal{R}(\Lambda)}\}$$

is finite.

From Lemma 1 and Lemma 2, if we denote by $\overset{\circ}{H} = \overset{\circ}{W}_{\mathcal{R}(\Lambda)} - \overset{\circ}{W}_{\mathcal{R}(\Lambda)}$, the symmetric object with respect to the origin, we deduce that the lower bound

$$\vartheta(\Lambda) = \inf\{\|\pi_{\parallel}(z - s)\| \mid z, s \in \Lambda, z - s \notin \mathbb{R}^{k-n} \text{ and } \pi_{\perp}(z - s) \in \overset{\circ}{H}\}$$

for the distance between two centres of spheres in $\mathcal{K}_{\mathbb{Q}}^k(\Lambda)$ is strictly positive. Therefore, we can take $r = \vartheta(\Lambda)/2$.

DEFINITION. With the above notations, we define

$$(15) \quad \gamma_{\mathbb{Q}}^{(k)}(\Lambda) = \frac{(\vartheta(\Lambda))^2}{(\text{disc}(\Lambda))^{1/k}}$$

and call $\gamma_{\mathbb{Q}, n}^{(k)} = \sup_{\Lambda} \gamma_{\mathbb{Q}}^{(k)}(\Lambda)$ the *Generalized Hermite function* associated with $G, n, \mathcal{R}, \{v_i\}, k$, the supremum being taken over all lattices Λ in $\mathbb{R}^k$.

It is not restrictive to consider only the lattices of determinant +1 in the above definition to define the supremum.

LEMMA 3. *We have*

$$(16) \quad \vartheta(\Lambda)^2 \leq m^{(k)}(\Lambda).$$

Indeed, if $x_{\min}$ denotes an arbitrary minimal vector of Λ , that is a vector x such that $m^{(k)}(\Lambda) = \langle x, x \rangle$, and $x_{\min} \notin \mathbb{R}^{k-n}$, we have $\vartheta(\Lambda) \leq \|\pi_{\parallel}(x_{\min})\| \leq \|x_{\min}\|$. If all the minimal vectors are located in $\mathbb{R}^{k-n}$, this is a fortiori true.

If Λ is extreme, that is such that $\gamma_k = \gamma^{(k)}(\Lambda)$, then the number of its minimal vectors will be greater than $k(k+1)/2$ [2, 42]. From Lemma 3, and

$$(17) \quad \gamma_Q^{(k)}(\Lambda) = \gamma^{(k)}(\Lambda) \frac{\vartheta(\Lambda)^2}{m^{(k)}(\Lambda)}$$

we deduce

PROPOSITION 2.

$$(18) \quad \gamma_{Q,n}^{(k)} \leq \gamma_n^{(k-1)/(n-1)}$$

PROOF. The Mordell-Rankin inequalities connecting γ_p and γ_{p+1} [43, 44]: $\gamma_{p+1} \leq \gamma_p^{p/(p-1)}$ for all integer $p \geq 2$ are applied to the sequence of Hermite constants: $\gamma_n, \gamma_{n+1}, \dots, \gamma_k$. This proves the inequality. $\square$

Here, n is fixed and k is variable. The upper bound $\gamma_n^{(k-1)/(n-1)}$ given by eq. (18) will be better if the periodization dimension k is chosen minimal. For some values of p , Rankin inequalities are known to be optimal, for other values, it is an open question [42].

4. Densities

The density $\delta(\Lambda)$ of a lattice Λ in $\mathbb{R}^k$ is connected to the function $\gamma^{(k)}(\Lambda)$ by the relation

$$(19) \quad \delta(\Lambda) = 2^{-k} v_k(1) \times (\gamma^{(k)}(\Lambda))^{k/2}$$

and the maximal density d_k (reached) in dimension k is linked to the Hermite constant γ_k by $d_k = 2^{-k} v_k(1) \gamma_k^{k/2}$. For quasiperiodic sphere packings, we expect such formulae with the generalized Hermite constant $\gamma_{Q,n}^{(k)}$ in a similar way. It is the case as proved in Theorem 1 below. If $\delta_Q^c(\Lambda)$, resp. $\delta_Q(\Lambda)$, denotes the centre density, resp. the density, of $\mathcal{K}_Q^k(\Lambda)$, we have

$$(20) \quad \delta_Q^c(\Lambda) = \limsup_{R \rightarrow +\infty} \left[\#(\{\pi_{\parallel}(c_i) | c_i \in \Lambda, \pi_{\perp}(c_i) \in \overset{\circ}{W}_{\mathcal{R}(\Lambda)}\} \cap \mathbb{B}_n(R)) / \text{vol}(\mathbb{B}_n(R)) \right]$$

and

$$(21) \quad \delta_Q(\Lambda) = \delta(\mathcal{K}_Q^k(\Lambda)) = \delta_Q^c(\Lambda) \times v_n(r(\Lambda))$$

THEOREM 1. *We have*

$$(22) \quad \delta_{Q,n}^{(k)} \leq \frac{\sup_{\Lambda, \det(\Lambda)=1} \left(\text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \right)}{\Gamma((n+2)/2)} \pi^{n/2} 2^{-n} (\gamma_{Q,n}^{(k)})^{n/2}$$

PROOF. The numerator of eq. (20) behaves like $\text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \times \text{vol}(\mathbb{B}_n(R))$ since the number of points of Λ in $\overset{\circ}{W}_{\mathcal{R}(\Lambda)} \times \mathbb{B}_n(R)$ is the same as in $\{\pi_{\parallel}(c_i) | c_i \in \Lambda, \pi_{\perp}(c_i) \in \overset{\circ}{W}_{\mathcal{R}(\Lambda)}\} \cap \mathbb{B}_n(R)$. Indeed, on one hand, after Rogers [45] and Cassels [46] we have: for $R \gg 1$ and any $\epsilon > 0$, there exists a lattice L in $\mathbb{R}^k$, of determinant $= 1$, such that

$$(23) \quad \sum_{\substack{x \neq 0 \\ x \in L}} \chi_R(x) < \int_{\mathbb{R}^k} \chi_R(x) dx + \epsilon$$

where χ_R is the characteristic function of the truncated cylinder $\overset{\circ}{W}_{\mathcal{R}(\Lambda)} \times \mathbb{B}_n(R)$ and is counting the elements of L inside this cylinder. On the other hand, after Remak [47], for any lattice L of determinant 1, there exists a point $z = z(L) \in \mathbb{R}^k$ such that

$$(24) \quad \sum_{\substack{z \in L \\ \det(L)=1}} \chi_R(x+z) \geq \int_{\mathbb{R}^k} \chi_R(x) dx$$

But any shift z does not change the centre density $\delta_Q^c(\Lambda)$, and we have

$$(25) \quad \int_{\mathbb{R}^k} \chi_R(x) dx = \text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \times \text{vol}(\mathbb{B}_n(R))$$

From eq. (21), and for any lattice Λ of determinant 1, we have

$$(26) \quad \delta_Q(\Lambda) \leq \sup_{\Lambda, \det(\Lambda)=1} \left(\text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \right) \times \sup_{\Lambda, \det(\Lambda)=1} (v_n(r(\Lambda)))$$

But

$$v_n(r(\Lambda)) = \pi^{n/2} r(\Lambda)^n / \Gamma((n+2)/2)$$

and

$$\gamma_Q^{(k)} = (2r(\Lambda))^2$$

since $\text{vol}(\Lambda) = \det(\Lambda) = \sqrt{\text{disc}(\overline{L})} = 1$. Hence,

$$\delta_Q(\Lambda) \leq \left(\sup_{\Lambda, \det(\Lambda)=1} \text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \right) \times \pi^{n/2} 2^{-n} (\gamma_{Q,n}^{(k)})^{n/2} / \Gamma((n+2)/2)$$

as announced. $\square$

Using Proposition 2, we obtain the upper bound as a function of n , k and a maximal window

COROLLARY.

$$(27) \quad \delta_{Q,n}^{(k)} \leq \frac{\sup_{\Lambda, \det(\Lambda)=1} \left(\text{vol}(\overset{\circ}{W}_{\mathcal{R}(\Lambda)}) \right)}{\Gamma((n+2)/2)} \pi^{n/2} 2^{-n} (\gamma_n)^{\frac{n(k-1)}{2(n-1)}}.$$

5. Discussion and examples

Among all the lattices $\Lambda \subset \mathbb{R}^k$, we have all the G -invariant lattices, since k is chosen on purpose for this (see §2). In the space $\mathbb{E}^n$ where quasiperiodic sphere packings are formed, the action of G is fixed (with ρ as in Proposition 1). When Λ is close in $GL(k, \mathbb{R})/GL(k, \mathbb{Z})$ to a $\bar{\rho}(G)$ -invariant lattice, the local configurations of spheres in $\mathcal{K}_Q^k(\Lambda)$ will become almost $\rho(G)$ -invariant with a certain frequency of occurrence. This comes from the definition of the selection scheme where, in eq. (13), the window can be made almost G -invariant in $\mathbb{R}^{k-n}$. The so-called core packings of Hsiang become predefinite, with predefinite frequencies of occurrence, in $\mathcal{K}_Q^k(\Lambda)$ by the window of eq. (12), what allows better upper bounds for the locally averaged densities, and by averaging as explained in the introduction, possible global better bounds than eq. (22) for the density. We have computed upper bounds for the density according to the reduction scheme $\mathcal{R}$. If we start from a unique lattice Λ to which several reduction theory are applied, we obtain several bounds which are linked to the possible optimal volumes of the windows, through eq. (27). We will report later on the influence of $\mathcal{R}$ on eq. (27). Let us recall that, whatever the positive integer n , γ_n^n is a rational number [2], and that only the values of γ_n are known for small values of n : for instance, for $n = 2, 3, 4, 5, 6, 7, 8$, we have $\gamma_n^n = 4/3, 2, 4, 8, 64/3, 64, 256$ [8] respectively.

In the plane and in space. In the context of Penrose tilings ($k = 6, n = 3$; or $k = 5, n = 2$), several models are explicetly described and it is possible to obtain fairly elevated densities by placing balls inside the prototiles (thick and thin rhombs in dimension 2; prolate and oblate rhombohedra in dimension 3) in a suitable way. We would like to recall some recent works and results, focusing essentially to the dimension 3, which were inspired by the coming of quasicrystals in the field of physics and chemistry, and the mathematical problems they involve for their modelling [27, 28].

In each case, in dimension 3, the conjectured bound $\pi/\sqrt{18} = 0.7404\dots$ is not reached, in any of the proposed models. In 1986, Henley [21] has started the study of quasicrystals in terms of occupation and densification schemes in the Penrose tiles, enumerating frequencies of occurrence of various local environments. Some *packing fractions* he obtains are 0.5535, 0.6288, $\dots$ starting from Λ one of the cubic lattices in $\mathbb{R}^6$: the simple cubic Λ_{SC} , the body cubic Λ_{BC} or the face centered cubic lattice Λ_{FCC} . Cockayne [48] proposed a Monte Carlo simulation to produce cubic approximant crystals of density 0.637, closely related to quasicrystals, not far from the density 0.64 of *random close packings* of spheres [49, 50, 51] as far as the terminology *random* is mathematically defined. An explicit quasiperiodic model of

quasicrystal was given by Ogney and Duneau [23] with *different* radii of spheres to simulate the *different* sizes of the atoms and relevant choices of windows, trying to fit their model to the observations. In this case, spheres have not the same radius. By considering similar objects packed quasiperiodically like spheres, Olami and Alexander [22] have proposed a method for maximizing the packing density from one of the lattices Λ_{SC} , Λ_{BC} , Λ_{FCC} , by enlarging as far as possible the corresponding window. A reduction scheme is here implicitly chosen for the lattices and explicit algebraic considerations allow to avoid too short distances in the quasiperiodic systems of spheres. The densities reached by such methods lie in the range 0.48 - 0.65. Such methods applied in dimension 2 [24] have demonstrated curious features which are easily generated by suitable optimal choices of windows, namely the existence of a very dense *backbone* of spheres surrounded by a *sea* of less well packed spheres, corresponding to the fact that the optimal Voronoi cell cannot tile $\mathbb{E}^3$ and generates 'defects'. Wills [25] has reconsidered this 2 dimensional approach by Olami and Kléman [24] to construct a 2+1 dimensional dense of quasicrystal, '2' for indicating that it is quasiperiodic in a plane and '1' for saying that it is periodic along the orthogonal direction, in the attempt to model so-called decagonal quasicrystals [28]. The density obtained is 0.67798, much higher than the previous ones. More directly in the way of constructing 2+1 dimensional quasiperiodic systems of spheres, Wills [26] has proposed sequences of systems of spheres in cylindrical 3 dimensional Penrose tilings whose densities tend towards 0.7341 ..., not far from Kepler's bound. New concepts recently appeared such as the notion of parametric density and its links to Wulff shapes, crystalline growth, ... [52, 53] to understand systems of spheres in crystallographic terms.

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